

N-(2-((1-(Cyclohexylmethyl)-2-(3-ethyl-2-oxo-5-oxazolidinyl)-2-hydroxyethyl)amino)-2-oxo-1-(2-thienylmethyl)ethyl)-gamma-oxo-alpha-(phenylmethyl)-4-morpholinebutanamide  
122225-00-7 | DTXSID80153548

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 15.1

Global applicability domain: Outside

Local applicability domain index: 1.55e-01

Confidence level: 6.71e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N,N',N',N",N"- Hexakis(methoxymethyl)-1,3,5- triazine-2,4,6-triamine</div> <div>Measured: 3.47</div> <div>Predicted: 4.50</div>	<div>Image not found</div> <div>Tris(2-butoxyethyl) phosphate</div> <div>Measured: 5.75</div> <div>Predicted: 6.32</div>	<div>Image not found</div> <div>Docusate sodium</div> <div>Measured: 9.33</div> <div>Predicted: 8.95</div>
<div>Image not found</div> <div>Tris(2-ethylhexyl) trimellitate</div> <div>Measured: 14.8</div> <div>Predicted: 40.7</div>	<div>Image not found</div> <div>Di(2-ethylhexyl) phthalate</div> <div>Measured: 589</div> <div>Predicted: 295</div>	